VIRTUAL CEMENT AND CONCRETE

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ABSTRACT

In the past, progress in cement and concrete science and technology has come mostly by deduction from the results of empirical investigations. As the body of knowledge about cement and concrete grows and becomes computerized, so does the possibility of relying more on induction to solve technological problems. In this speculative paper, it is suggested that we can look forward to the not-far-distant day when the performance of cements in concrete will be able to be predicted from knowledge of measured properties of the cement and other constituents, the mixture proportions, and the expected conditions of mixing, curing, and use. It will then be possible to conceive of a cement that has not yet been made -- a "virtual cement" -- and predict the performance of a "virtual concrete" made with it. The resulting ability to investigate the effects of possible changes in the composition and particle size and shape distribution of a cement quickly and cost-effectively will have broad impacts. It should facilitate product development.

KEYWORDS: cement; concrete; databases; expert systems; integrated knowledge systems; simulation models; standards; sustainable technology; virtual technology

INTRODUCTION

Looking to the 21st Century, the authors believe that the confluence of many factors will cause rapid growth in the contents and usefulness of computerized knowledge bases, including those for cement and concrete [1], and construction in general. The computerization of knowledge will be among the most important of technological developments because of the pervasiveness of its impacts; it will benefit most technologies, including those of cement and concrete.

To provide the context for a discussion of emerging technologies pertaining to cement and concrete, it will be useful to begin with speculations about likely changes in materials-related aspects of the construction knowledge base. Referring to Figure 1(a), the construction cycle [2] is represented in the outer circle, while the inner circle and its contents represent the materials knowledge drawn on in making decisions in the construction cycle. Near the end of the 20th Century, the knowledge is in the form of the related, but only loosely connected, items indicated in the inner circle -- research results, texts, data, expert opinion, anecdotal information, and standards. Some of the knowledge comes from laboratory research, and some from observations in the field. The arrows between the inner and outer circles indicate whether the knowledge base is likely to be drawn upon (outward-pointing arrow) or added to (inward-pointing arrow) in the various phases of the construction cycle. The circle labelled "codes" (meaning building codes) is also part of the materials knowledge base, but it is shown separately because codes may act more as filters for knowledge from the other sources.

Figure 1(b) is our view of how Figure 1(a) should be redrawn to show the construction materials knowledge as we expect it to be early in the 21st Century. The materials knowledge in the inner circle is now a computerized integrated knowledge system consisting of research results, databases, knowledge-based expert systems, and standards shown as concentric rings to indicate they are part of a purposefully designed system; the lines between the rings are broken to indicate that there are no real barriers between the parts of the computerized system. While Figure 1(b) has similarities to (a), the knowledge in the knowledge base of 1(b) will be of much greater value because it will be more complete and easier to use. The result should be higher quality and more quickly made decisions in the construction process.

The inner circles of Figures 1(a) and 1(b) could be taken to represent the state of organization of knowledge of either or both of cement and concrete as it exists today in 1995, (a), and as emerging technologies might make it in, say, 2005, (b). At this point it will be helpful to discuss the generation of results from cement research between now and about 2005. At present, our knowledge of cement science and technology is being increased by addition of individual increments ("nuggets") of knowledge. For the most part, the areas covered by the individual nuggets of knowledge do not coalesce. However, when enough nuggets bearing on different but related aspects of a subject coalesce, they may help define a new or expanded technology. It is suggested that, by 2005, research will have made the nuggets of knowledge regarding cement science and technology grow to the extent that many more will have coalesced, thereby allowing predictions of performance to be made routinely and, possibly, helping define some new technologies. If the subject area covered includes many complementary simulation models, it could define a "virtual" technology encompassing more than a technology based on experiment alone.

In the case of the research and development (R&D) process, changes taking place as the 21st Century approaches may be represented as in Figure 2 (which is based on a figure in Reference 3). Figure 2(a) shows the traditional R&D process in which an hypothesis (or concept or theory) is tested by experiment and, depending on the results, the hypothesis may be revised and the cycle repeated until satisfactory agreement with experiment is obtained. The usual output from the R&D activity is data and text (papers and reports). Figure 2(b) shows the developing R&D process in which the hypothesis is formulated and then modelled mathematically, with the model being subjected to testing against data from experiments which are increasingly computer-assisted -- the computer assistance being in one or more of planning, implementation (increasingly with automation), and analysis; the outputs from the process are increasingly in the form of databases, simulation models, and text which could become elements of an integrated knowledge system such as that depicted in Figure 1(b). This raises critical questions for potential beneficiaries of an integrated knowledge system. In the cement and concrete context, the questions are such as: Should the growth of an integrated knowledge system for cement (and concrete) be planned? And if so: By whom?

When? How? And what should be the scope? And looking further ahead: How should an integrated knowledge system for cement (and concrete) be maintained? How should the quality of its contents be controlled and protected? And how should it be paid for?

The sorts of questions listed here are not purely academic. The authors believe that a serious attempt must soon be made to answer them. They also believe that the search for answers to the questions would disclose important opportunities for the industry and the nation. It is a purpose of this paper to try to show the nature of the opportunities.

FACTORS MAKING DEVELOPMENT OF AN INTEGRATED KNOWLEDGE SYSTEM FOR CEMENT AND CONCRETE FEASIBLE

The authors believe that many factors that will make possible rapid growth in the content and usefulness of the cement and concrete knowledge base at the start of the century are already apparent. To continue the speculations, we expect developments resulting from these factors will greatly increase the confidence with which scientific and technological decisions about cement and concrete can be made. Such decisions may, for example, be about how to formulate a concrete with a specific performance, or how long a specific concrete product will last in a given environment. Among factors which are already having an effect individually and are starting to act in concert are:

- Advances in materials science and recognition that cement and concrete are worthy of study by materials scientists [4]
- Growing recognition of possibilities for raising the performance of concrete and other cementitious materials to new levels in one or more important performance attributes such as strength, durability, toughness, ease of placement, and dimensional stability [5]
- Results being generated in national high-performance concrete programs in many countries [6]
- Increases in the power and availability of computers [3]
- Advances in communications capability (the "information superhighway") [7]
- Advances in materials characterization capability [8]
- Development of computerized databases [9]
- Development of knowledge-based expert systems [10]
- Development of the computational materials science of cement and concrete (simulation models) [11]

The last three of these make possible computerized representations of knowledge of cement and concrete that will complement each other and will be able to be linked to form <u>integrated knowledge systems</u>. The systems will have the capability of making useful predictions of the performance of cement and concrete -- predictions that until recently were outside the bounds of practicality. The capability of performance prediction is called for by the Civil Engineering Research Foundation (CERF) in its proposed national "High-Performance Construction Materials and Systems Program" [6], and it is also a goal of the National

Science Foundation's Center for the Science and Technology of Advanced Cement-Based Materials (ACBM) [12] (see Figure 3 which shows computer-based modelling and archival databases as integrating factors for the outputs from research in the surrounding topical areas). Performance predictions are needed to optimize concrete and other cementitious materials for high-performance applications and for exploring possibilities for using nontraditional cementing materials in concrete in support of the movement towards sustainable technology ("green technology" [13]). The goal would be to base the predictions, as far as possible, on the properties of the constituents, and the concrete processing conditions, and the service conditions.

In cases in which the performance predictions are for materials that have not yet been produced (as they might often be), the materials will be referred to as "virtual", as opposed to "real." We think it self-evident that virtual cement and concrete technology will be valuable, provided it is practical to use it to make decisions of technical and economic importance that could not reasonably be made without it.

In the remainder of this paper we shall show the feasibility of developing a virtual cement and concrete technology based on ability to make performance predictions and review some implications of virtual cement and concrete technology. It will be seen that there are implications for many aspects of the manufacture and use of concrete and concrete materials, including quality control and quality assurance, condition assessment and repair (of concrete), standards and codes, education and training, innovative materials, and innovative uses of materials.

In our opinion, the ability to make realistic predictions of the long-term performance of virtual cements and concrete without carrying out a large number of lengthy experiments is possible and will soon be achieved. This is in accord with the paradigm illustrated in Figure 2(b) [3]. Among the benefits will be accelerated progress in cement and concrete technology as a result of ability to investigate, in less than real time, the effects of changes in almost any parameter affecting concrete performance, even though it might take months or years to obtain the same insight by physical experiments. Indeed, it should be possible to investigate the implications of some changes in cement and concrete characteristics that cannot yet be reliably measured, e.g., subtle inhomogeneities (flaws) in concrete, or distribution of phases among particles in a cement. The predictions should be particularly valuable in providing insights into complex multivariable problems in which physical experiment would be considered too costly or too time-consuming. Examples of problems that virtual cement and concrete technology should be able to address are suggested in the next section.

TYPES OF QUESTIONS THAT VIRTUAL CEMENT AND CONCRETE TECHNOLOGY SHOULD HELP ANSWER

To illustrate the importance of developing ability to investigate the properties performance of virtual concrete and other virtual cementitious materials, it is relevant to note that, at present, many questions of potential technological importance go unanswered (or do not even get posed explicitly) because it appears that it would be too costly to try to answer them by the physical experimental route. Examples of such questions are:

- o Of all the available portland cements, which would be the best for use in a concrete for a specific application?
- o If it could be made, what would be the characteristics of the optimum portland cement (or blended cement) for a given application?
- o Will a proposed concrete mixture last 500 years in the expected service environment?
- o For a portland cement of a specified phase composition to be used in a given application of concrete, what would be the optimum size and shape distribution of the particles and how would the phases be distributed among the particles?
- o If a phase (such as calcite, quartz, silica fume, tetracalcium trialuminate sulfate , or a glass such as that in a fly ash or a granulated blastfurnace slag) from outside the portland cement range in the C-A-S-F system were to be used to modify the portland cement resulting from the previous question, what would be the optimum amount to be added and how could it and should it be distributed among the particles?
- o How sensitive is the performance of a cement in a given application to small changes in phase composition? Particle size distribution? Particle shape distribution?
- o How sensitive is the performance of a concrete in a given application to changes in the processing conditions? Environmental conditions? Aggregate composition, and size and shape distributions? Admixture composition, concentration, and time of addition?

The answers to such questions could lead to improvements in the manufacture and use of cements and concrete. For example, they could help advance high-performance concrete technology, and they could be useful in helping optimize concretes to meet many demands, e.g., economy, conservation of resources, or environmental impact ("greenness"). Part of the problem is the difficulty in defining performance in quantitative terms, often because the needed methods of measurement have not yet been developed. In such cases, the best that can done at present is to rely on the scientific and technical intuition of an expert. However, if validated tools for investigating the properties of virtual cements and concretes were available, rapid progress should be possible because "What if ...?" questions would be able to be answered quickly and with confidence. Simulation models developed in the Cementitious Materials Modelling Laboratory (CMML) [14] in the Building And Fire Research Laboratory (BFRL) at the National Institute of Standards and Technology (NIST) indicate the possibilities. (The CMML is a joint activity of NIST and the National Science Foundation's Center for Science and Technology of Advanced Cement-Based Materials.)

PROGRESS TOWARDS VIRTUAL CEMENTS AND CONCRETES AND PREDICTION OF THEIR PERFORMANCE

In research in the CMML, often carried out in collaboration with researchers from other organizations, several models with potential for use in the investigation of virtual cements and concretes have been developed in steps directed towards the construction of a comprehensive model for performance simulation and prediction. They include chemical models for the hydration of individual spherical particles, and assemblies of spherical particles, of C_3S and C_3A [15], and, most recently, pixel-based digital techniques for representation of the microstructures of hardening portland cement pastes of various phase compositions, with and without mineral admixtures, and for calculating physical and mechanical properties of the hardened cement pastes [16]. While a comprehensive model is not yet in place, enough has been done to show the potential of the virtual cement and concrete concept, and continuing research at NIST and in other laboratories throughout the world is providing new knowledge which will contribute to the model. An example is the work of Nonat on factors affecting the kinetics of hydration of C_3S [17]. While the reaction kinetics cannot yet be predicted by the present NIST model, virtual experiments can be carried out in which multiphase particles of different shapes and sizes are packed in a volume to represent different water/(cementitious material) (w/cm) ratios and stages in the formation of the microstructure during the course of the cementing reactions can also be displayed. Further, properties of the hardened paste can be calculated as a function of the degree of hydration of the cement. Model calculations give insights into the effects of particle size distribution, w/cm ratio, and degree of hydration on such aspects of the performance of virtual cement pastes as elastic modulus, time of set, shrinkage, diffusivity, transport within the pore structure, and rheological properties.

In extending the simulations from virtual cements to virtual concretes, substantial computational problems are having to be overcome. The problems result from the much larger volume needed to represent a concrete. A volume of the order of 100 cm^3 needed to represent a typical concrete is about 10^5 times as large as the volume of about 0.001 cm^3 needed to represent a typical cement paste. This suggests that if the same pixel-based digital representation is to be used for cement paste and concrete, about 10^5 times as much computer memory will be needed for dealing with concrete. At present, this is not practical so, in an alternative approach [18], the concrete is represented as aggregate dispersed in a paste represented as a continuum and with an interfacial transition zone around each aggregate particle; the properties of the paste and interfacial zone are then calculated separately using a "cement paste/sand grain" model [19]. This multi-scale approach has allowed modelling of the diffusivity of cement paste [20] to be extended to mortar and concrete. Pixel-based calculations have given insights into the structure of cement pastes in the interfacial transition zones around individual aggregate particles in a mortar and the conditions under which percolation of interfacial transition zones around sand grains will occur. These insights have helped explain the results of mercury intrusion experiments on mortars with different sand/cement ratios [21].

With the continually increasing range and sophistication of models for simulation of aspects of the performance of mortars and concretes, the authors believe that there should be no property of practical importance that cannot be predicted with sufficient accuracy to be useful. A sketch to show the relationships that can already be seen to be developing among virtual and real cement and concrete systems is presented in Figure 4 (from Reference 22). The sketch indicates how images of particulate materials can be used to obtain computer-generated (virtual) microstructures which, when combined with particle property data, can be used in calculations of the properties of the hardened cement-based material.

As the range of models grows, it is to be expected that the models, or results obtained from their use, will be incorporated into user-friendly decision-support systems that continue to evolve and become more powerful. For example, it is possible that the HWYCON expert system mentioned in the next section could be the first stage in an always-complete, yet continually-evolving, increasingly-powerful, decision-support system formed by incorporation of a progression of increasingly sophisticated and realistic models that take advantage of the continued growth in the power and speed of computers and the sizes of their memories.

THE KNOWLEDGE SYSTEM NEEDED TO EXPLOIT VIRTUAL CEMENT AND CONCRETE TECHNOLOGIES

At present, the practicality and usefulness of techniques for investigating virtual cements and virtual concretes is limited by the amount of knowledge of cement and concrete stored in, or accessible by, computers. The rate of growth of the knowledge base will undoubtedly increase due to demands such as those for support of virtual cement and concrete technology and other needs of the information age. The needed knowledge will consist of data (including stored images), simulation models, and knowledge-based expert systems, with the data being in standardized sets and formats. Progress being made in all of these categories is setting the stage for an explosion of activities when all the parts can be put together in an integrated knowledge system accessible through the Internet [7].

The current state of affairs is that some necessary developments are taking place in all the needed forms of computerized knowledge. Standards for representation of concrete material property data that, among other uses, will aid simulations of the properties and performance of virtual cements and concretes are being drafted by ACI Committee 126 on Concrete Material Property Data; the recommended formats are consistent with guidelines prepared by ASTM Committee E49 on Computerization of Material and Chemical Property Data [23]. Simulation models needed for representation of virtual cements are being developed by NIST, in conjunction with other members of the NSF Center for Science and Technology of Advanced Cement-Based Materials (ACBM), and these are being shared with ASTM Committee C01 on Cement through its Research Subcommittee. And a pioneering knowledge-based expert system to aid technical decisions concerning concrete has been developed by NIST, as part of a project led by the Construction Technology Laboratories under the Strategic Highway Research Program (SHRP); the expert system is named HWYCON [24]. Although HWYCON was developed to apply specifically to concrete in highway structures and pavements, it is capable of expansion to include other applications of concrete. It provides an early example of the implementation of an expert system for concrete, with 3000 copies being made available by the Transportation Research Board.

An integrated knowledge system composed of parts such as those mentioned in this section would be a representation of virtual cement and concrete technology. Among the many useful purposes it would serve would be education at many levels, including guidance in the development and use of logically-consistent cement and concrete standards.

VIRTUAL CEMENT AND CONCRETE TECHNOLOGY AND STANDARDS FOR CEMENT AND CONCRETE

It is generally recognized that prescriptive standards, while convenient for quality control, can be barriers to innovation, and that performance standards are needed to reduce or remove the barriers. It is also recognized that performance standards that require long-term tests (e.g., over periods of months or years) are not suitable for routine use. For this reason, at least at present, both prescriptive and performance standards for cement (and concrete) are still needed, though, for the future, it seems likely that predictive standards in which the performance of a cement could be predicted from the cement's properties could serve the purposes of both [25]. This would be an important application of virtual cement technology.

Validated performance prediction models should be valuable in helping rationalize cement and concrete standards. Whereas the present standards have, for the most part, been developed on an as-needed, empirical basis, it should be possible to analyze the needs and see which existing standards should be kept or improved, which should be replaced, and what new ones should be added to make the set as coherent and as useful as possible. It may be that some standards could be enhanced or replaced by standardized, knowledge-based expert systems.

The fact that interactive electronic presentations of standards is now possible offers new opportunities for improving dissemination of standards knowledge. For example, the main text of a standard in electronic form could be backed up by interactive explanatory materials with different depths of detail that could be called upon by the user as needed. The benefits could be particularly great in the case of complex standards such as ACI 318, Building Code Requirements for Reinforced Concrete, if the commentary were in the form of a knowledge-based expert system.

In view of the need to consider performance standards for cement in terms of the application, the present ASTM system in which cement standards are developed in one ASTM committee (ASTM C-1) and standards for most other concrete materials are developed in another (ASTM C-9) should be reviewed to see if a different subdivision of responsibilities between the committees, or a closer collaboration, as through joint activities or a merger, should be sought. As has been pointed out by Hooton in an editorial article [26], it does not seem rational to develop standards for some cementing materials (e.g., ground, granulated blastfurnace slag) in one committee and those for portland and blended cements in another.

Among new types of standard that may be needed to support technological advances in cement, other concrete materials, and concrete, are standard predictive models, standard formats for data sets, and standard knowledge-based expert systems. In addition, new standard test methods are likely to be needed for performance characteristics of special importance in high-performance concrete technology. As an example, the need to reduce water/cementitious material (w/cm) ratios from the traditional levels to obtain the benefits that low porosities can bring to strength and durability suggests that there may be a need for improved tests of the rheological properties governing the flow of cementitious materials. In addition, the desirability of being able to predict performance suggests there should be standard methods of test for new properties needed as input to the performance prediction calculations; possible examples are standards for i) phase analysis of cements, ii) particle size and shape distribution of cements and other particulate ingredients, and iii) rate of heat evolution.

CONDITION ASSESSMENT AND REPAIR (OF CONCRETE)

The integrated knowledge system for cement and concrete that can be foreseen should include assistance with identifying causes and mechanisms of distress and the selection of repair materials and procedures. The HWYCON system [24] that already exists suggests the possibilities. Plans for extending the scope of HWYCON to include concrete in general, not only concrete in highway bridges and pavements, are being formulated.

EDUCATION AND TRAINING

Predictive tools are likely to have an important role in enhancing the knowledge of civil engineers and materials scientists about cement and concrete. In any case, professionals who work with cement and concrete will need to be familiar with the tools that can introduce them to cement and concrete technology at a greater depth than before. The predictive tools will also be useful for presenting the knowledge, at any appropriate depth, to any person in the cement and concrete technology chain -- a building inspector, structural engineer, concrete technologist, cement plant chemist, laboratory technician, field technician, construction specifier, or "do-it-yourselfer" -- since the interactive format will lend itself to tailoring to meet needs at the different levels, whether for formal classes or home study. Examples of pioneering efforts in disseminating information about the developing tools are the ACBM/NIST annual workshop on computer modelling and the educational module on the computational materials science of cement-based materials that NIST has prepared under the auspices of the ACBM [27]. The growth in content of the ACBM/NIST modelling workshop from year to year shows how rapidly developments are taking place.

The computer-aided education could logically be extended to include cement and concrete knowledge systems (which could, themselves, be an integral part of the education process) and standards and codes.

INNOVATIVE MATERIALS AND USES

The predictive capability of virtual technology need not be limited to conventional cement and concrete. For example, a model has already been developed for MDF (macro-defect free) cement [28]. In this case, to help explain the transport properties in the composite formed from calcium aluminate cement, water, and polyvinyl alcohol or other water-soluble resin, a "hard core/soft shell" model was developed. It is expected that more comprehensive models for MDF cements will be developed, and that models for other new cementitious materials such as DSP (cement densified with small particles) [29], fiber-reinforced cement, and polymer concrete will be developed, and that the models will deal with whatever properties are of likely technical or commercial interest, e.g., electrical or electronic properties, toughness, crack initiation and growth, or ease of extrusion.

SUMMARY

Of all the developments that will influence cement and concrete technology in the 21st Century, virtual cement and concrete technology is likely to be among the most important. Virtual cement and concrete technology are being made possible by advances in materials science (specifically computational materials science), increases in the power and availability of computers, and development of "the information superhighway." The virtual technology will be manifested in the form of integrated knowledge systems (decision support systems) consisting of complementary simulation models, databases, an10d knowledge-based expert systems. It will bring a new level of technical decision-making capability to the cement and concrete industries.

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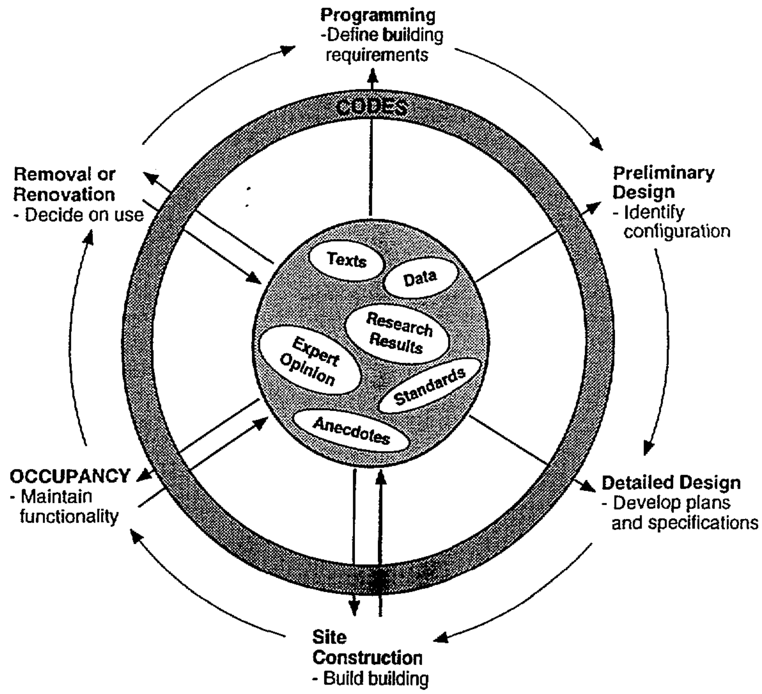
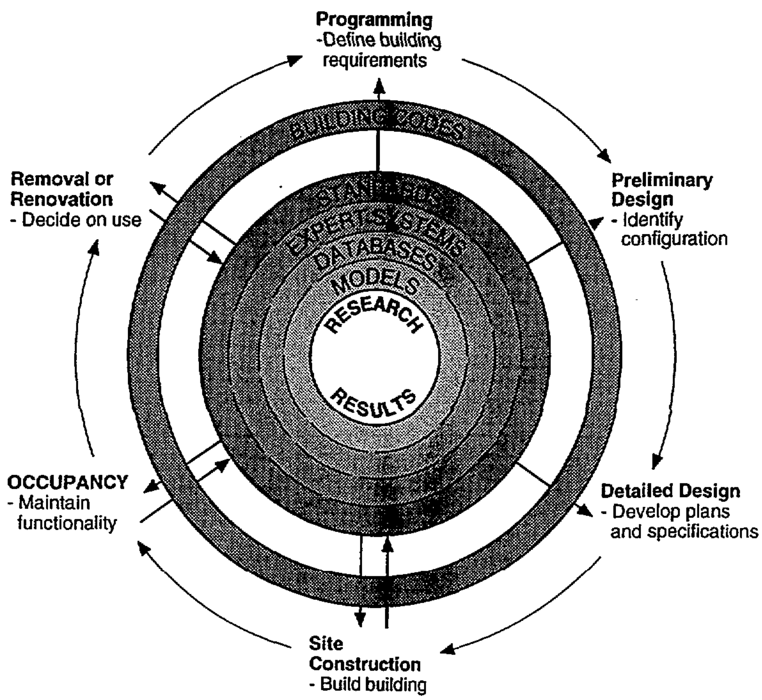
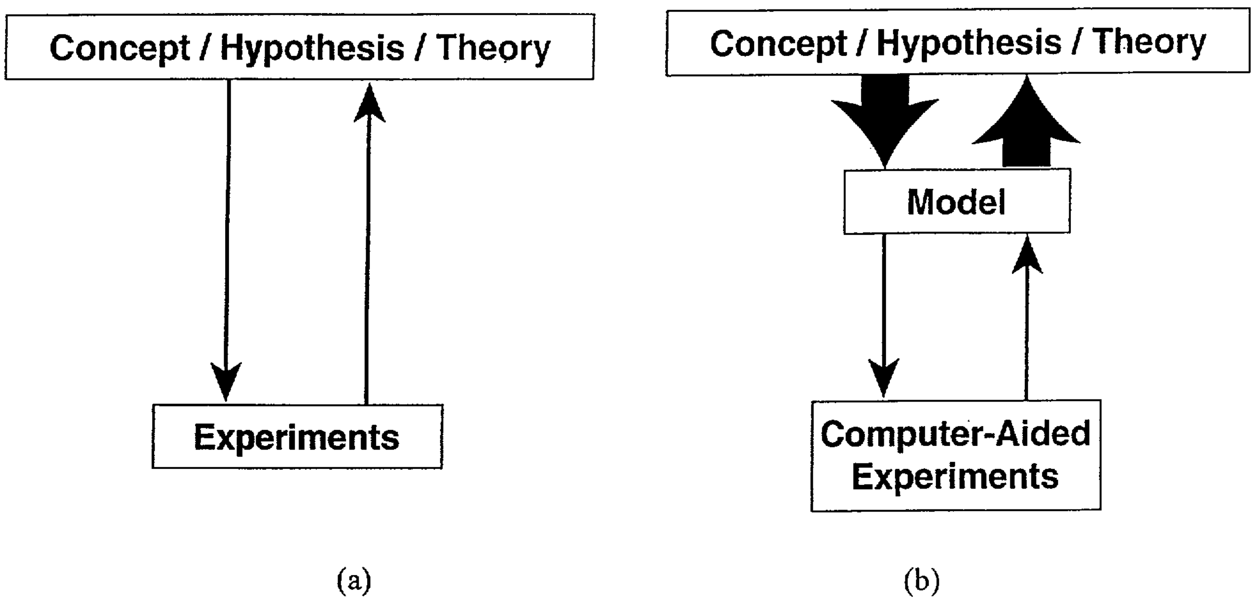


a) Late 20th century -- forms of knowledge are not integrated

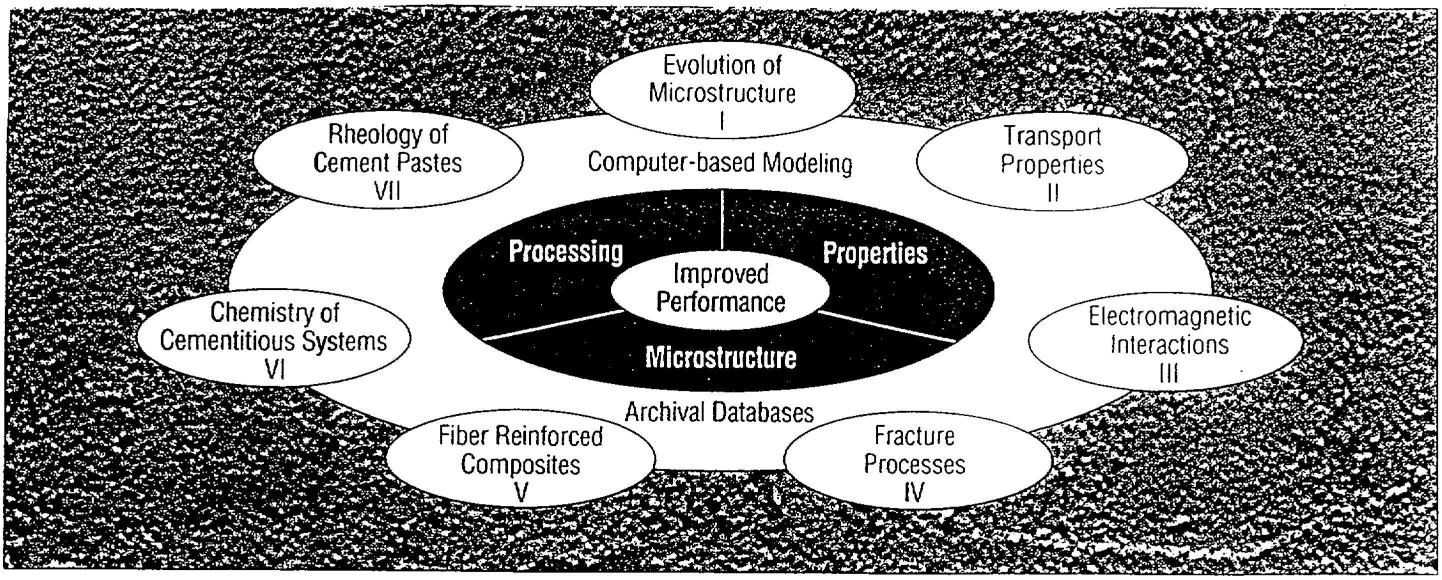


b) Early 21st century -- knowledge is computer-integrated

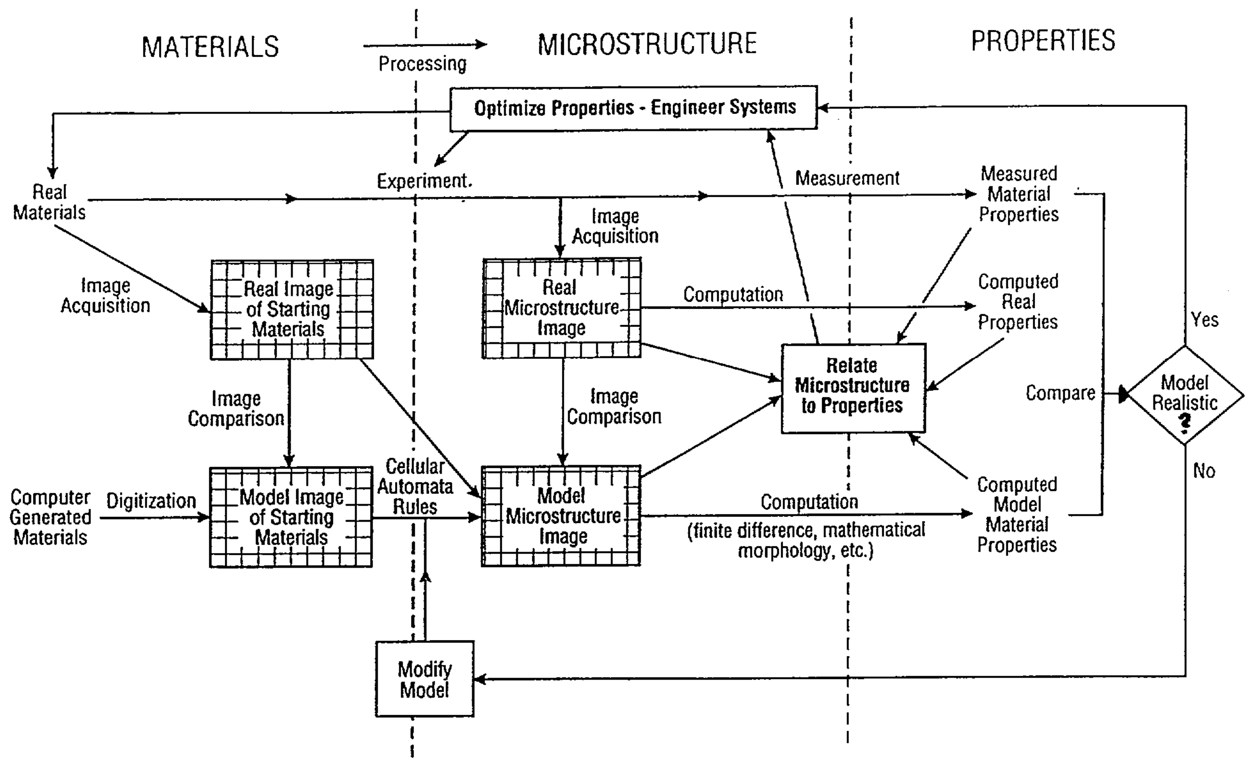
Fig, 1. Materials knowledge and the construction cycle



Fig, 2. The R&D process: a) late 20th century, b) early 21st century (based on a figure in [3]).



Fig, 3. The research structure of the Center for Advanced Cement-Based Materials [12] showing computer-based modeling and archival databases as integrating factors.



Fig, 4. Flow chart indicating how images of particulate materials can be used to obtain virtual, computer-generated microstructures and to calculate properties of hardened cement-based materials (a slightly modified figure from [22]).